

Journal of Magnetic Resonance

EDITOR: Wallace S. Brey, Jr.

EDITORIAL BOARD:

E. Raymond Andrew
Edwin D. Becker
James W. Cooper
Richard Ernst
Ray Freeman
J. H. Goldstein
David M. Grant
R. K. Harris

James S. Hyde
Charles S. Johnson, Jr.
J. Jonas
Robert Kaptein
Lowell Kispert
Gerd La Mar
George C. Levy
Ralph Livingston

Bruce McGarvey
Henry A. Resing
Rex E. Richards
A. Rigamonti
Ian C. P. Smith
E. O. Stejskal
Robert L. Vold
D. E. Woessner

Volume 52, 1983



ACADEMIC PRESS

A Subsidiary of Harcourt Brace Jovanovich, Publishers

New York London

Paris San Diego San Francisco São Paulo Sydney Tokyo Toronto

Copyright © 1983 by Academic Press, Inc.

All Rights Reserved

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owner.

The appearance of the code at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients. This consent is given on the condition, however, that the copier pay the stated per copy fee through the Copyright Clearance Center, Inc. (21 Congress Street, Salem, Massachusetts 01970), for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Copy fees for pre-1983 articles are as shown on the article title pages; if no fee code appears on the title page, the copy fee is the same as for current articles.

0022-2364/83 \$3.00

MADE IN THE UNITED STATES OF AMERICA

CONTENTS OF VOLUME 52

NUMBER 1, MARCH 1983

A. A. SHUBIN AND S. A. DIKANOV. The Influence of Nuclear Quadrupole Interactions upon Electron Spin-Echo Modulation Induced by Weak Hyperfine Interactions	1
KEISAKU KIMURA. A New Formalism of Chemical Exchange near the Region of Intermediate Rate	13
PETER A. SEHR, COLIN MAILER, AND PHILIPPE F. DEVAUX. Saturation Transfer Dispersion Electron Paramagnetic Resonance Using a Balanced Cavity: Dynamical Calibration and Biological Applications	23
AD BAX, THOMAS A. EARLY, AND GARY E. MACIEL. Proton Chemical Shifts in Polycrystalline Solids Determined by Off-Resonance Decoupling ¹³ C CP-MAS NMR	35
B. BLÜMICH AND D. ZIESSOW. Practice of Multidimensional Stochastic NMR Spectroscopy. The Derivation of 1D, 2D, and 3D Spectra	42
A. G. AVENT, J. W. EMSLEY, AND DAVID L. TURNER. NMR Spin-Echo Spectra of Molecules Containing Four Spin-1/2 Nuclei with AA'BB' Symmetry in Liquid-Crystalline Samples	57
M. MAĆKOWIAK AND R. J. C. BROWN. Pressure Dependence of ¹⁹ F Spin Relaxation in (NH ₄) ₂ SiF ₆	71
AD BAX. A Simple Method for the Calibration of the Decoupler Radiofrequency Field Strength	76
M. ROBIN BENDALL, DAVID T. PEGG, AND DAVID M. DODDRELL. Pulse Sequences Utilizing the Correlated Motion of Coupled Heteronuclei in the Transverse Plane of the Doubly Rotating Frame	81
NOTES	
PETER J. SMOLENAERS, M. TERRY KELSO, AND JAMES K. BEATTIE. A Sensitive ¹³ CMR Shift Thermometer Using Dysprosium Ion in Acetate Buffer	118
J. BORNAIS, S. BROWNSTEIN, AND S. BYWATER. Elimination of Solvent Signals in Carbon Magnetic Resonance Spectroscopy	120
JACOB SCHAEFER, R. A. MCKAY, AND E. O. STEJSKAL. Dipolar Rotational Spin-Echo ¹³ C NMR of Polymers	123

G. WIDER, R. V. HOSUR, AND K. WÜTHRICH. Suppression of the Solvent Resonance in 2D NMR Spectra of Proteins in H ₂ O Solution	130
M. R. BENDALL AND D. T. PEGG. Reexamination of a Sequence Designed to Cancel ¹³ C Signals of Protonated Carbons	136
KEITH MORGAN, BRIAN G. SAYER, AND GARY J. SCHROBILGEN. Bismuth NMR Spectroscopy: ²⁰⁹ Bi and ¹⁹ F High-Resolution NMR Spectra of the Hexafluorobismuthate(V) Ion	139
M. D. PACE AND B. S. HOLMES. Spin Trapping of •NO ₂ Radicals Produced by uv Photolysis of RDX, HMX, and Nitroguanidine	143
COMMUNICATIONS	
AD BAX, NIKOLAUS M. SZEVERENYI, AND GARY E. MACIEL. Correlation of Isotropic Shifts and Chemical Shift Anisotropies by Two-Dimensional Fourier-Transform Magic-Angle Hopping NMR Spectroscopy	147
C. A. G. HAASNOOT. Selective Solvent Suppression in ¹ H FT-NMR Using a DANTE Pulse: Its Application in Normal and NOE Measurements	153
A. J. SHAKA, TOM FRENKIEL, AND RAY FREEMAN. NMR Broadband Decoupling with Low Radiofrequency Power	159
M. ROBIN BENDALL AND DAVID T. PEGG. EPT with Two Variable Pulse Angles, a Universal Polarization Transfer Sequence	164
NUMBER 2, APRIL 1983	
T. A. BABUSHKINA, V. F. ZOLIN, AND L. G. KORENEVA. Interpretation of Lanthanide-Induced Shifts in NMR Spectra. The Case of Nonaxial Symmetry	169
S. K. HOFFMANN AND L. S. SZCZEPANIAK. Dynamical Averaging of Two Symmetry-Related Magnetic Resonance Tensors in Single Crystals . . .	182
J. JOKISAARI, P. DIEHL, J. AMREIN, AND E. IJÄS. Solvent Dependence of Deuteron Quadrupole Coupling Constants and of Methyl Angles of Some CD ₃ X Compounds Determined by NMR of Partially Oriented Molecules	193
KERRY K. KARUKSTIS AND PETER SMITH. INDO-MO Study of δ-CH Acetyl-Proton Couplings in Aliphatic α-Acetoxy Radicals	202
C. P. KEIJZERS, T. JANSEN, E. DE BOER, G. VAN KALKEREN, AND J. S. WOOD. The Nature of the Jahn-Teller Effect in the Copper-Doped Hexaimidazole Zinc Dichloride Tetrahydrate Complex	211
MARK RANCE AND R. ANDREW BYRD. Obtaining High-Fidelity Spin-1/2 Powder Spectra in Anisotropic Media: Phase-Cycled Hahn Echo Spectroscopy	221

J. C. WALTON. The ^{13}C Hyperfine Splittings in ESR Spectra of Prop-2-ynyl and 1-(Trimethylsiloxy)prop-2-ynyl Radicals	241
E. E. BABCOCK AND J. H. GOLDSTEIN. Structure and Orientation of Propargyl Chloride Partially Oriented in a Nematic Mesophase	247
PAUL D. ELLIS, PING P. YANG, AND ALLEN R. PALMER. Cadmium-113 NMR Spin-Lattice Relaxation and Exchange Kinetics in Concanavalin A: A Double Saturation Transfer Experiment	254
N. SCHUFF AND U. HAEBERLEN. 2D Correlation Spectroscopy in Homonuclear Dipolar-Coupled Solids	267
LARRY WERBELOW. Nuclear Magnetic Resonance Flip-Angle Effects: Observability of Multipole Operators	282

NOTES

GEORGES BRAOUDAKIS, IOANNIS P. GEROTHANASSIS, AND JÜRGEN LAUTERWEIN. Calculation of Transverse Relaxation Times from Lineshapes Modified by Gaussian-Exponential Filtering	288
REINO LAATIKAINEN. How Restricted Are Partially Restricted MO Calculations? A Few Comments on the Calculations of Spin-Spin Coupling Pathways at the INDO/FPT Level	293
D. HORNE, R. D. KENDRICK, AND C. S. YANNONI. Bond Length Measurements in Amorphous Solids by Nutation NMR Spectroscopy: The Role of rf Field Homogeneity	299
R. NUNLIST AND J. D. ARENIVAR. A Simple Method for Simultaneous Homo- and Heteronuclear Decoupling on FT-NMR Spectrometers	305
RENÉ RICHARZ AND H. SAUTER. ^{13}C Shift Anisotropies in Polycrystalline Calcium Formate	308
ALFRED G. REDFIELD. Fast and Economical Treatment of 2D NMR Data	310
ROBERT W. DYKSTRA. A Broadband Radiofrequency Reflected-Wave Detector and Its Application to a Nuclear Magnetic Resonance Spectrometer	313
N. P. LUTHRA, R. B. DUNLAP, AND J. D. ODOM. The Use of Dimethyl Selenide as a Chemical Shift Reference in ^{77}Se NMR Spectroscopy	318

COMMUNICATIONS

A. DULČIĆ AND B. RAKVIN. Frequency Versus Field Modulation in Magnetic Resonance	323
PHILIP H. BOLTON. Heteronuclear Zero Quantum Spectroscopy as a Conformational Probe	326

AD BAX. Determination of Heteronuclear Coupling Constants via Semi-Selective Two-Dimensional J Spectroscopy	330
A. J. SHAKA, JAMES KEELER, TOM FRENKIEL, AND RAY FREEMAN. An Improved Sequence for Broadband Decoupling: WALTZ-16	335
P. J. HORE, R. M. SCHEEK, AND R. KAPTEIN. Multiplet Selection Using Multiple Quantum Coherence	339
P. DUBOIS MURPHY. Improvement in the Cross-Polarization NMR Experiment for Suppression of Rigid Protonated Carbons	343
DAVID L. FOXALL AND JACK S. COHEN. NMR Studies of Perfused Cells	346

NUMBER 3, MAY 1983

STEVE C. F. AU-YEUNG AND DONALD R. EATON. Chemical Shift Anisotropy and Second-Sphere Hydrogen Bonding in Cobalt (III) Complexes	351
STEVE C. F. AU-YEUNG AND DONALD R. EATON. The Solvent and Field Dependence of ^{59}Co NMR Linewidths	366
GARY TOMLINSON. Transient Effects in Homonuclear Double Resonance	374
J. R. PILBROW, G. R. SINCLAIR, D. R. HUTTON, AND G. J. TROUP. Asymmetric Lines in Field-Swept EPR: Cr^{3+} Looping Transitions in Ruby	386
VYACHESLAV A. CHERTKOV AND NICKOLAY M. SERGEYEV. ^{13}C Isotope Effects on the Parameters of Proton Magnetic Resonance Spectra of Benzene	400
M. ROBIN BENDALL, DAVID T. PEGG, AND DAVID M. DODDRELL. Comparison of Decoupling and Spatial Randomization Methods for Use in Editing ^{13}C Spectra	407
R. A. WIND, F. E. ANTHONIO, M. J. DUIJVESTIJN, J. SMIDT, J. TROMMEL, AND G. M. C. DE VETTE. Experimental Setup for Enhanced ^{13}C NMR Spectroscopy in Solids Using Dynamic Nuclear Polarization	424
SANDRA S. EATON, KUNDALIKA M. MORE, BHIMRAO M. SAWANT, PAUL M. BOYMEL, AND GARETH R. EATON. Metal-Nitroxyl Interactions. 29. EPR Studies of Spin-Labeled Copper Complexes in Frozen Solution	435
V. MACHO, R. KENDRICK, AND C. S. YANNONI. Cross Polarization Magic-Angle Spinning NMR at Cryogenic Temperatures	450
J. R. MORTON AND K. F. PRESTON. EPR Spectroscopy of Single Crystals Using a Two-Circle Goniometer	457
J. I. KAPLAN AND K. V. VASAVADA. A Numerical Calculation of the NMR Lineshape Using the Finite Difference Method	475

DAVID P. KELLY, D. RALPH LESLIE, AND ROBERT A. CRAIG. Carbon-13 Spin-Lattice Relaxation Mechanisms for the t-Butyl Cation in Superacid. Importance of Chemical Shift Anisotropy to the Relaxation of Cationic Carbons	480
---	-----

NOTES

EINAR SLETTEN, J. TIMOTHY JACKSON, PHILLIP D. BURNS, AND GERD N. LA MAR. Effects of Cross Relaxation on the Analysis of T_1 Data in Paramagnetic Proteins	492
PETER SCHMITT AND HARALD GÜNTHER. Assignment of ^{13}C Resonances and $^{13}\text{C}, \text{X}$ Spin-Spin Coupling Constants via Double-Quantum Coherence	497

COMMUNICATIONS

JOSEPH H. BATTOCLETTI AND RICHARD E. HALBACH. Optimal Field for Detection of Magnetically Labeled Blood	500
ZHONG-XIAN HUANG AND GEOFFREY R. MOORE. Variation of NMR Chemical Shifts Induced by $[\text{Fe}(\text{CN})_6]^{3-}$	505
PETER SCHMITT, JOACHIM R. WESENER, AND HARALD GÜNTHER. ^{13}C Spin-Echo Modulation through $^{13}\text{C}, ^2\text{H}$ Spin-Spin Coupling: Elimination of Solvent Signals and Analysis of Partially Deuterated Systems	511
R. B. CREEL. Analytic Solution of Fourth Degree Secular Equations: $I = \frac{3}{2}$ Zeeman-Quadrupole Interactions and $I = \frac{7}{2}$ Pure Quadrupole Interaction	515
T. E. GLASS AND H. C. DORN. A High Sensitivity Toroid Detector for ^{17}O NMR	518
DAVID M. DODDRELL, JAMES STAUNTON, AND ERNEST D. LAUE. Multipulse Techniques to Edit ^{13}C NMR Spectra of Deuterated Compounds. Useful Methods to Follow Deuterium in Biosynthesis ...	523
J. C. EVANS AND P. H. MORGAN. Simulation of Electron Spin Resonance Spectra by Fast Fourier Transform	529

AUTHOR INDEX FOR VOLUME 52	532
----------------------------------	-----

The Subject Index for Volume 52 will appear in the December 1983 issue as part of a cumulative index for the year 1983.

